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Vacancy-induced Relaxations in Er_3Si_5

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Erbium silicide has attracted recent attention because it is a metallic conductor that is nearly lattice-matched to silicon, and because it forms well-ordered epitaxial layers on the Si (111) surface. There has also been considerable interest in dilute alloys of Er in Si for more than a decade because the Er luminescence at 1.54 μm , corresponding to the minimum in absorption of silica-based optical fibers, offers the promise of applications in optoelectronics. The structure of these dilute alloys is poorly understood. A more detailed understanding of bulk Er_3Si_5 and the factors determining its structure should provide guidance in studying these alloys.

The structure of erbium silicide is a superstructure of the primitive hexagonal AlB_2 structure. It consists of a hexagonal lattice of Er atoms centered over the hollow sites of graphitic layers of Si, giving a hypothetical stoichiometry of ErSi_2 . The observed stoichiometry of the most stable bulk material, however, is Er_3Si_5 , which is consistent with one of every six atoms in each Si layer missing. Recent work has shown that the Si vacancies are rotated 120° in alternate Si planes as one proceeds up the c axis, yielding ABAB stacking, see Fig. 1. A series of density functional calculations was carried out to understand the driving forces giving rise to the formation of these vacancies and the structural relaxation they induce. The calculated structure yielded lattice parameters that were within 1% of powder x-ray diffraction measurements. Internal relaxations relative to the hypothetical ErSi_2 structure are substantial, with the 3 Si around the vacancy moving inward an average of 0.43 Å. Such distortions result in a broad distribution of Er–Si bond lengths, 2.88 - 3.32 Å. The individual bond lengths, unavailable from the powder diffraction data, were used as input for a simulated EXAFS spectrum, which was in excellent agreement with experiment. Comparison with the hypothetical ErSi_2 structure showed that the vacancies provide more efficient metallic bonding between the Er atoms by allowing the Si atoms to form flat rather than buckled layers.

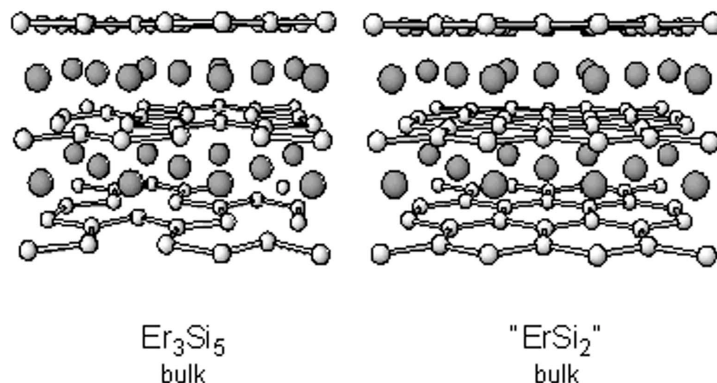


Figure 1. Comparison between the most stable Er silicide structure containing Si vacancies, Er_3Si_5 , and the hypothetical ErSi_2 structure. For clarity, bonds between Er (dark balls) and Si are omitted